SUPPLEMENTARY INFORMATION

on

Tribological investigations of β-lactum cephalosporin antibiotics as efficient ashless antiwear additives with low SAPS and their theoretical studies

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S1. Experimental details

The wear scar diameter of each of the three horizontal balls was measured in two mutually perpendicular directions, one in the sliding direction (d_s) and the other perpendicular (d_p) to it using an optical microscope. Geometric mean of the two perpendicular diameters on the same ball was taken as given by the equation 1.

For each experiment arithmetic mean of the above diameter of each ball (d_1,d_2 and d_3) was taken as given by equation 2. The three stationary balls were not disturbed while taking the readings and the wear scar diameter was taken by tilting eye piece of the microscope at an angle of 70.5^0 making it perpendicular to the surface of the scar.

S1.1 Tribological Parameters

S1.1.1 Mean wear scar diameter (MWD)

$$d_1 = \sqrt{(d_s d_p)} \tag{1}$$

$$d = \frac{d_1 + d_2 + d_3}{3} \tag{2}$$

S1.1.2 Mean wear volume (MWV)

Wear volume, $$V = \frac{\Pi \, d_0^4}{64 \, r}\{(\frac{d}{d_0})^4 - (\frac{d}{d_0})\} \tag{3}$$

Hertzian diameter, $$d_0 = 2(\frac{3Pr}{4E})^{\frac{1}{3}}$$

Where, $$\frac{1}{r} = \frac{1}{r_1} + \frac{1}{r_2}$$

$$\frac{1}{E^*} = \frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2}$$

Where, E^* = Resultant modulus of elasticity

v = Poissons ratio

r = Radius of steel ball

$E_1 = E_2 = 206$ GPa

$v_1 = v_2 = 0.3$

P = Actual load in Newton on each of the three horizontal balls that is 0.408 times of applied load.

S1.1.3 Friction coefficient (μ)

The coefficient of friction for different antiwear additives is calculated from the pattern observed on the friction paper with the help of equation 4.

$$\mu = \frac{0.222F}{r} \cdot \frac{L}{P} \qquad 4$$

L/P = 0.628

r = 0.367 mm

$$F = \frac{springcons \tan t}{6} \times Y$$

Where, F = Friction force in kgf exerted on the indicator spring.

L = Length in mm of the torque-lever arm.

r = Distance of contact surface of balls from the axis of rotation (0.367 mm).

Y = Displacement after 2.5 s from the baseline.

Value of spring constant upto 80 kgf is 0.226 kgf/cm.

S1.1.4 Wear rate

Overall, running-in and steady-state wear rate have been calculated on the basis of observed mean wear volume data at different time intervals. Mean wear volumes at different times (15,

30, 45, 60, 75 and 90 min.) for each experiment were plotted with time and a linear regression model was fitted on the points including origin to find out overall wear rate.

$$\frac{V}{l} = K\frac{P}{H}$$

V = mean wear volume

l = sliding distance ($2\pi r.N$)

K = wear coefficient

H = hardness of steel ball (59-61 HRC)

P = applied load (0.408x392N)

S1.2 AFM Roughness Parameters

S1.2.1 Line Roughness:

Roughness Average, $R_a = \frac{1}{N}\sum_{l=0}^{N-1}|z(x_l)|$

Root Mean Square, $R_q = \sqrt{\frac{1}{N}\sum_{l=o}^{N-1} z(x_l))^2}$

Peak-Valley Height, $R_y = A_p - A_v$

Peak-Height, R_p = Highest value

Valley Depth, R_v = Lowest value

Mean Value, $R_m = \frac{1}{N}\sum_{l=0}^{N-1} z(x_l)$

S1.2.2 Area Roughness:

Roughness Average, $S_a = \frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}|z(x_k, y_l)|$

Root Mean Square, $S_q = \sqrt{\frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1}(z(x_k, y_l))^2}$

Peak-Valley Height, $S_y = S_p - S_v$

Peak-Height, $S_p =$ Highest value

Valley Depth, $S_v =$ Lowest value

Mean Value, $S_m = \frac{1}{MN}\sum_{k=0}^{M-1}\sum_{l=0}^{N-1} z(x_k, y_l)$

Table S1. Tribological parameters for paraffin oil in the presence and absence of β–lactum antiwear additives (1% w/v) for different time duration at 392N applied load

S.N.	Additive	Time (min)											
		15		30		45		60		75		90	
		MWD (mm)	MWV (10^{-4} mm^3)	MWD (mm)	MWV (10^{-4} mm^3)	MWD (mm)	MWV (10^{-4} mm^3)	MWD (mm)	MWV (10^{-4} mm^3)	MWD (mm)	MWV (10^{-4} mm^3)	MWD (mm)	MWV (10^{-4} mm^3)
1.	Paraffin oil	0.622	20.548	0.703	34.829	0.735	42.152	0.781	54.177	0.815	64.647	0.929	111.280
2.	ZDDP	0.411	02.698	0.556	12.457	0.594	16.821	0.630	21.728	0.678	29.843	0.685	31.184
3.	Cefixime	0.469	05.525	0.510	08.333	0.551	11.924	0.580	15.078	0.619	20.117	0.661	26.758
4.	Cephalexin	0.479	06.143	0.578	14.846	0.642	23.587	0.679	30.032	0.703	34.829	0.742	43.695
5.	Cefadroxil	0.471	05.645	0.531	10.078	0.581	15.113	0.613	19.275	0.647	24.394	0.681	30.412

MWD= Mean wear scar diameter, MWV = Mean wear volume

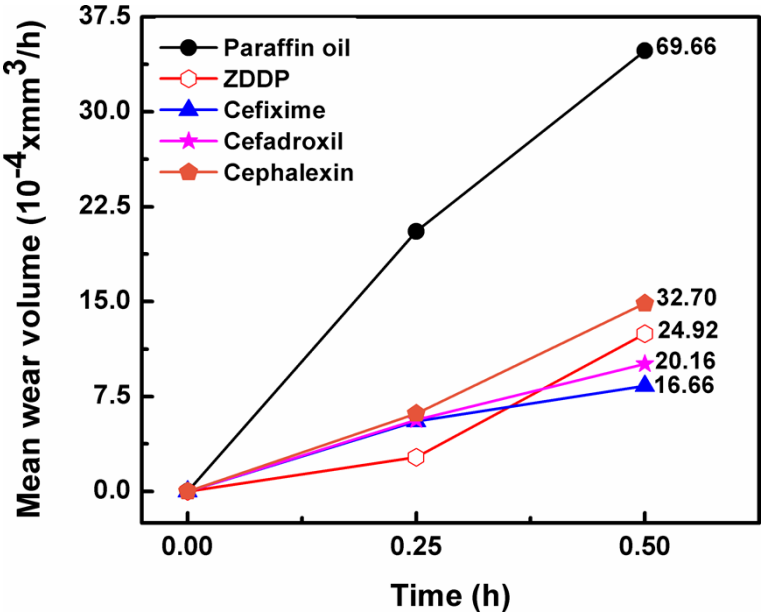


Fig. S1. Determination of running-in wear rate by varying mean wear volume with time (h) in paraffin oil containing (1% w/v) zinc dibutyldithiophosphate and β–lactum additives at 392N applied load

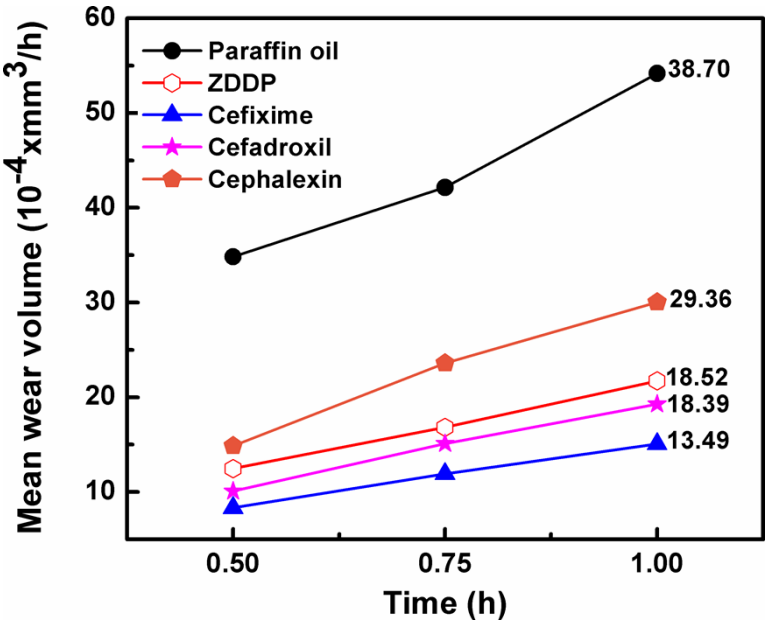


Fig. S2. Determination of steady-state wear rate by varying mean wear volume with time (h) in paraffin oil containing (1% w/v) zinc dibutyldithiophosphate and β-lactum additives at 392N applied load

Table S2. Tribological parameters for paraffin oil in the absence and presence of β-lactum antiwear additives (1% w/v) at different loads and for 30 min test duration.

S.N.	Additive	Applied Load (N)											
		294		392		490		588		686		784	
		MWD (mm)	μ	MWD (mm)	μ	MWD (mm)	μ	MWD (mm)	μ	MWD (mm)	μ	MWD (mm)	μ
1.	Paraffin oil	0.622	0.180	0.699	0.187	0.744	0.190	Fails					
2.	ZDDP	0.499	0.150	0.566	0.160	0.622	0.165	0.6440	0.180	Fails			
3.	Cefixime	0.469	0.135	0.491	0.142	0.502	0.149	0.5190	0.154	0.590	0.157	0.6128	0.180
4.	Cefadroxil	0.468	0.142	0.491	0.153	0.524	0.158	0.5606	0.161	0.611	0.172	0.7370	0.193
5.	Cephalexin	0.502	0.165	0.522	0.169	0.539	0.172	0.5850	0.178	0.633	0.192	Fails	

MWD= Mean wear scar diameter, μ= friction coefficient

Fig. S3a

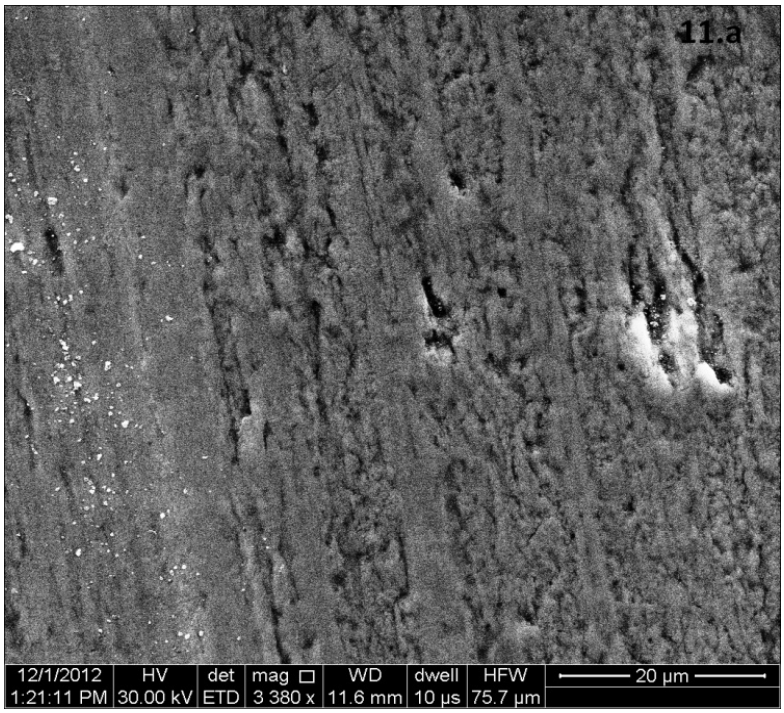


Fig. S3b

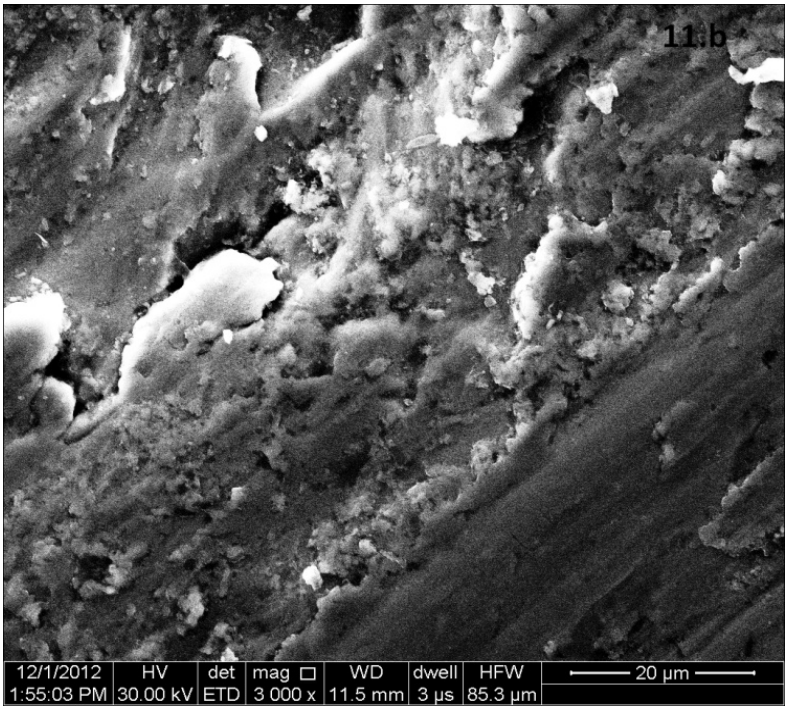


Fig. S3. SEM micrographs of the worn steel surface lubricated with, (a) cefixime and (b) ZDDP (1% w/v) in paraffin oil for 30 min test duration at 588 N applied load

Fig. S4a

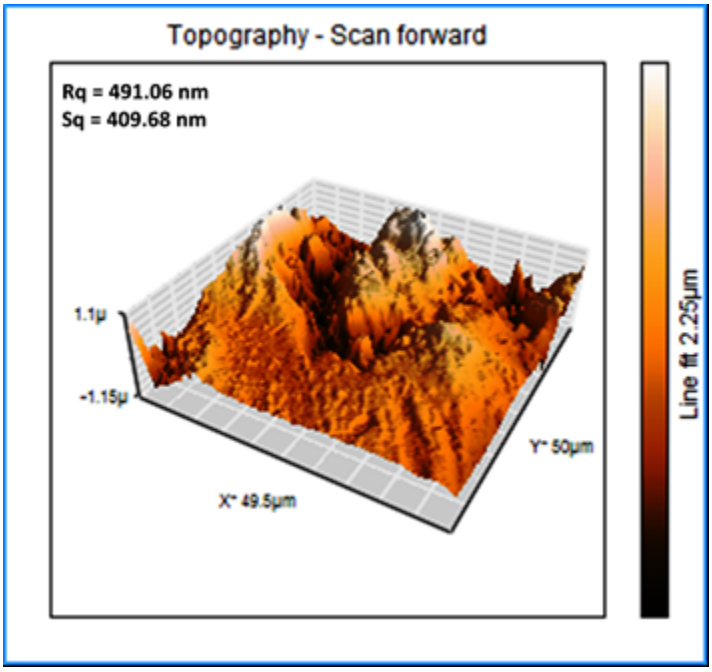


Fig. S4b

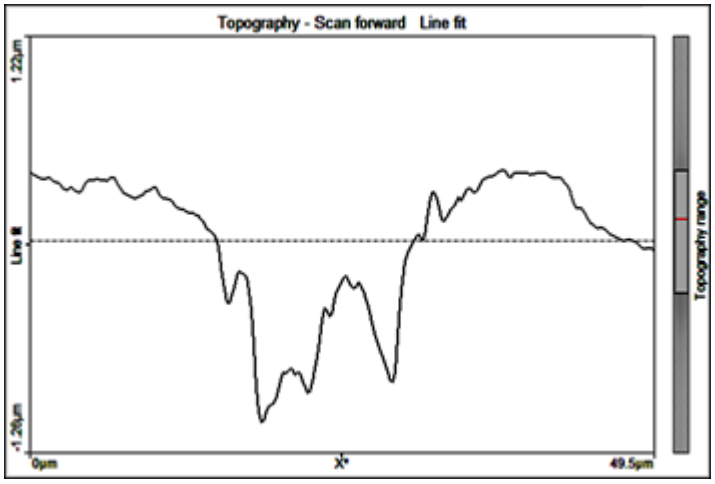


Fig. S4c

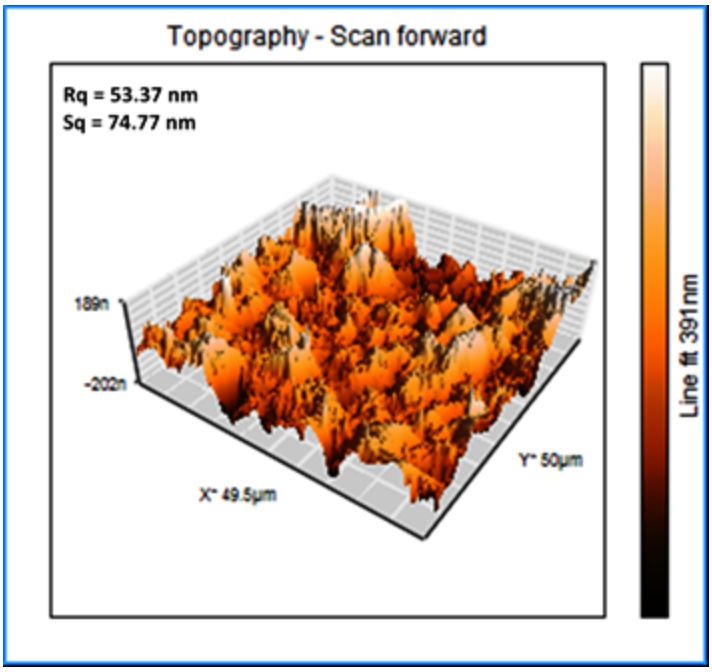


Fig. S4d

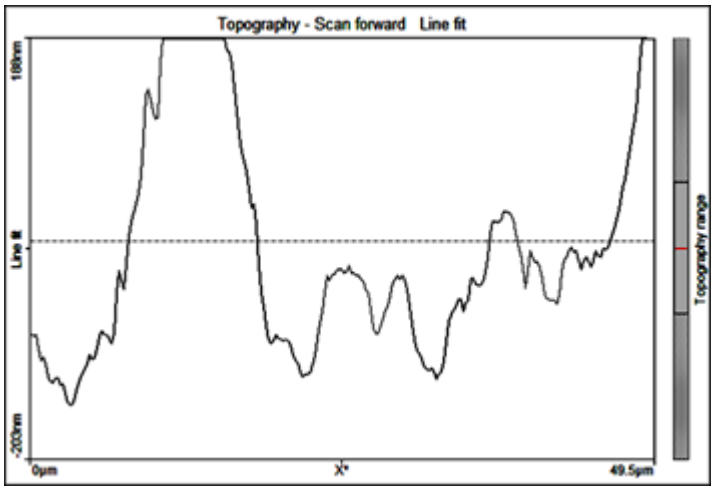
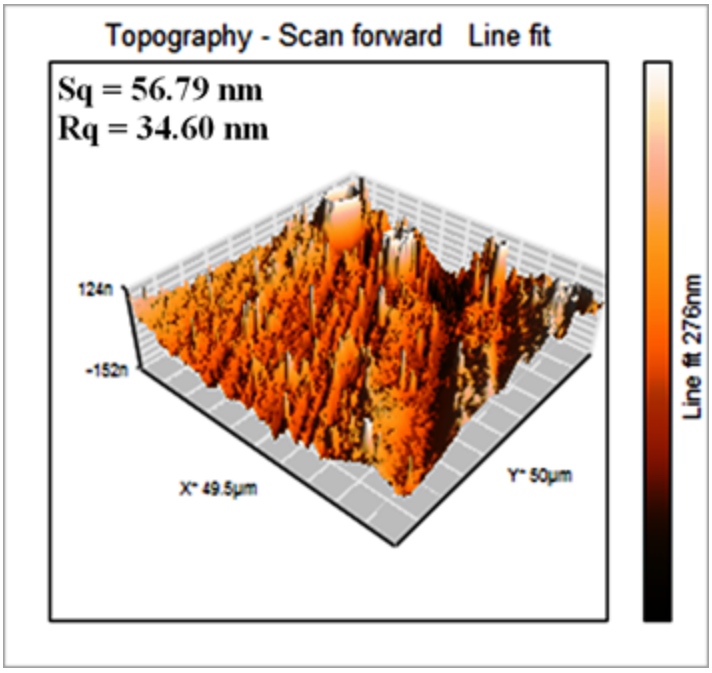


Fig. S4e



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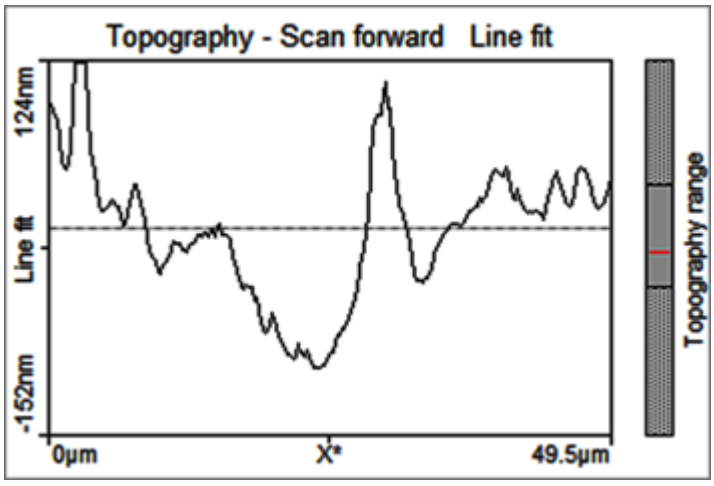

Fig. S4g

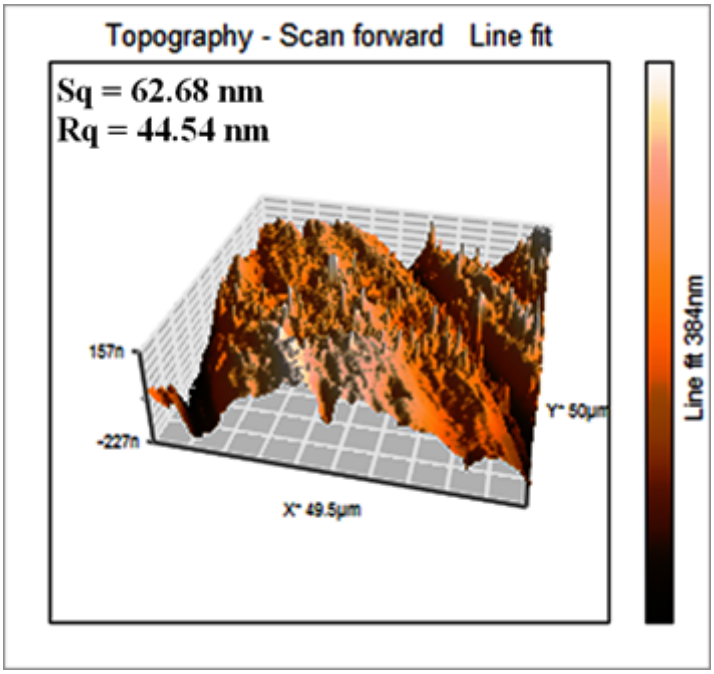

Fig. S4h

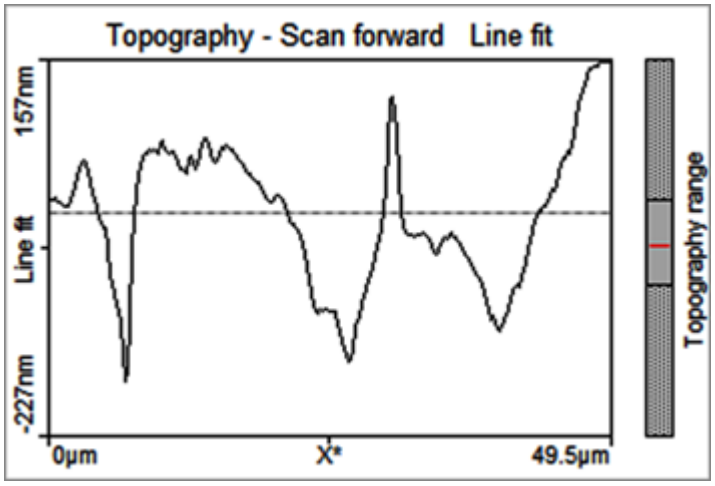

Fig. S4i

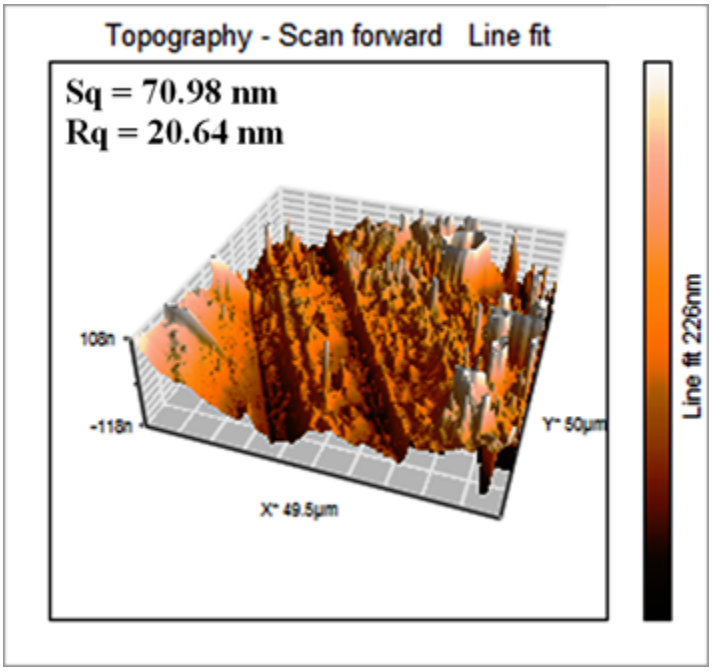

Fig. S4j

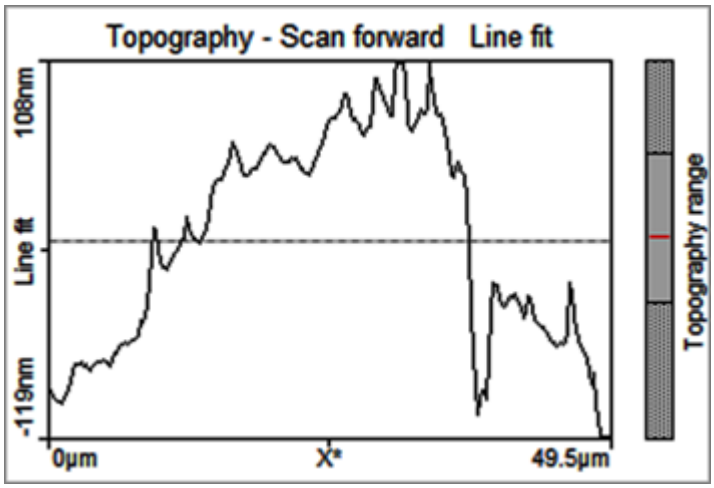

Fig. S4. 3*D*-AFM images and corresponding line profile graphs of the worn steel surface lubricated with β–lactum additives (1% w/v) in paraffin oil for 90 min test duration at 392 N applied load: (a,b) Paraffin oil, (c,d) Zinc dibutyldithiophosphate, (e,f) Cefixime, (g,h) Cefadroxil and (i,j) Cephalexin

Table S3. Surface Roughness parameters obtained from digital processing software of Nanosurf-basic Scan 2 for paraffin oil with and without additives at 392 N load for 90 min test duration.

Roughness Parameters	Paraffin oil	ZDDP	Cefixime	Cefadroxil	Cephalexin
Area Roughness 2.496 nm^2					
Sa	298.03nm	56.24nm	35.43nm	46.53nm	56.79nm
Sq	409.68nm	74.77nm	56.79nm	62.68nm	68.60nm
Sy	2.63µm	635.20nm	926.51nm	508.64nm	517.15nm
Sp	1153.30nm	369.75nm	741.26nm	250.39nm	294.91nm
Sv	-1471.70nm	-265.45nm	-185.15nm	-258.25nm	-222.24nm
Sm	174.66pm	111.74pm	143.6pm	128.73pm	150.75pm
Line Roughness					
Ra	422.98nm	38.97nm	28.84nm	33.30nm	61.11nm
Rq	491.06nm	53.37nm	34.60nm	44.54nm	74.12nm
Ry	1568.70nm	272.98nm	176.97nm	245.27nm	309.42nm
Rp	713.49nm	151.87nm	114.31nm	117.37nm	187.62nm
Rv	-855.20nm	-121.11nm	-62.65nm	-127.89nm	-121.80nm
Rm	-167.91pm	-215.64pm	-185.81pm	-195.19pm	-178.14pm

Fig. S5a

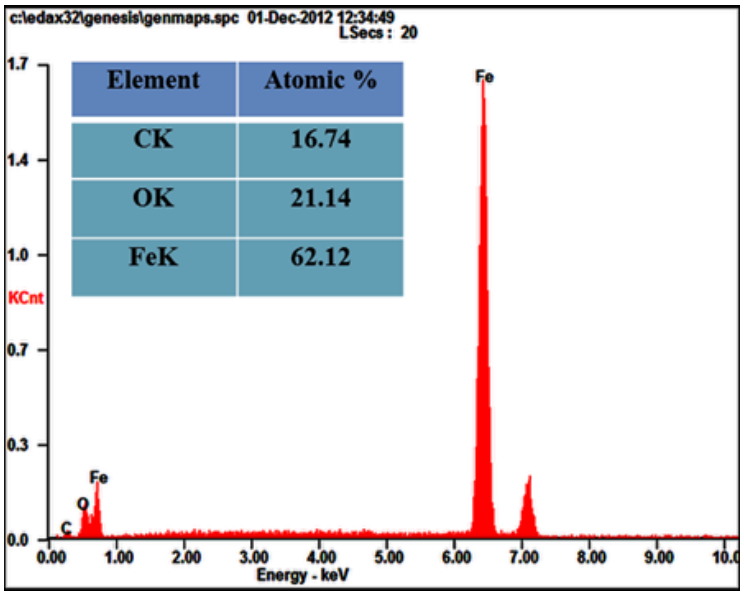

Fig. S5b

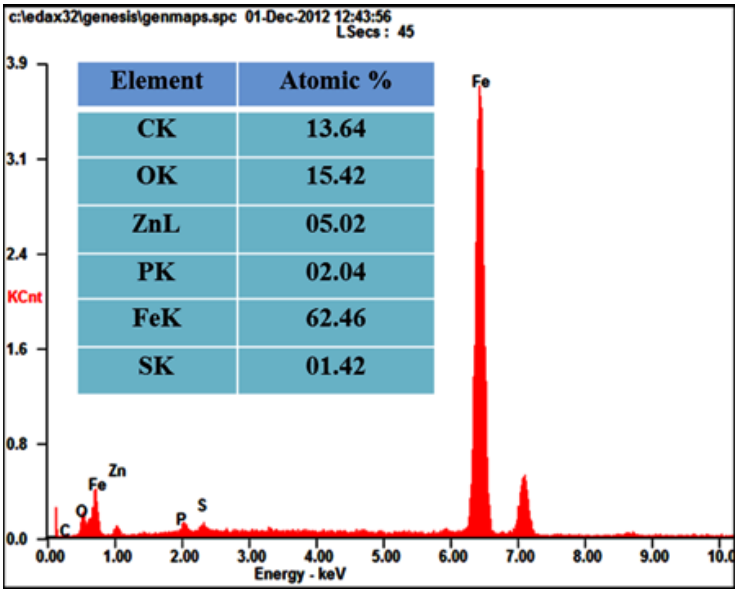

Fig. S5c

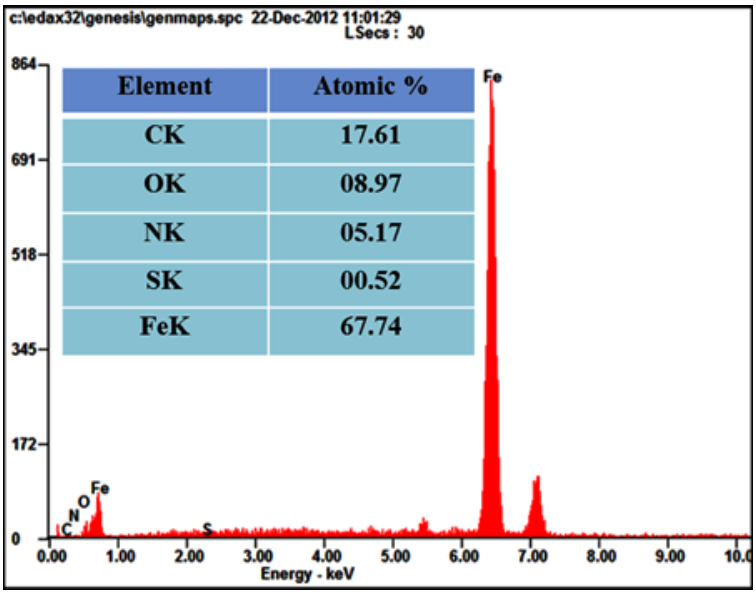

Fig. S5. EDX analysis data of the worn steel surface lubricated with paraffin oil in presence and absence of additives (1% w/v) for 90 min test duration at 392 N applied load: (a) Paraffin oil, (b) Zinc dibutyldithiophosphate (ZDDP) and (c) Cefixime

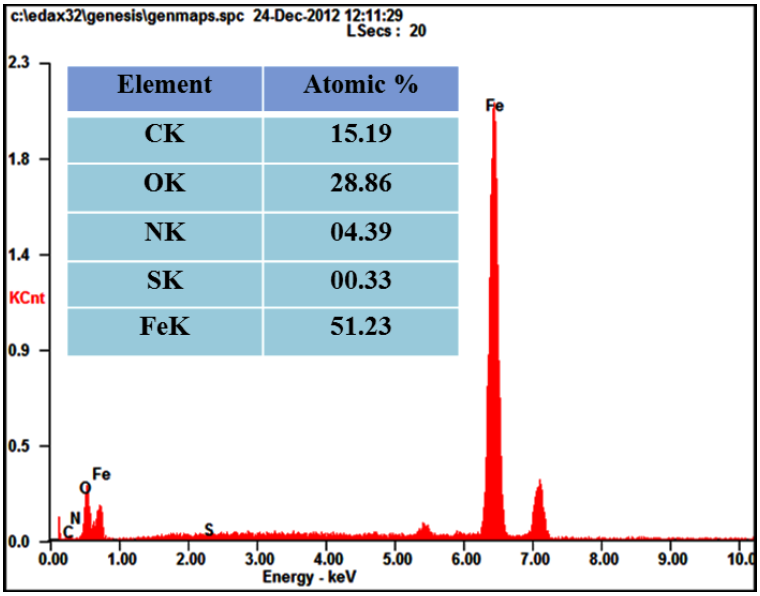

Fig. S6. EDX analysis data of the worn steel surface lubricated with paraffin oil in presence cefixime additives (1% w/v) for 30 min test duration at 588 N applied load